

Renumbered
claims

Amendment to the Claims:

This listing of claims will replace all prior versions, and listing, of claims in the application.

Listing of Claims:

1. (previously presented) A computer implemented method of generating standardized representative three dimensional conformations of the molecular side_chains derived from reactant molecules comprising the steps of:

- a) defining a set of topomeric alignment rules; and
- b) applying the topomeric alignment rules to the molecular side chains to generate a representative conformation for each.

2. (canceled)

23. (previously presented) A computer implemented method of characterizing the three dimensional structure of the molecular side chains derived from reactant molecules, which can assume many conformations, comprising the steps of:

- a) generating standardized representative three dimensional conformations of the molecular side chains derived from reactant molecules comprising the steps of:
 - (1) defining a set of topomeric alignment rules; and
 - (2) applying the topomeric alignment rules to the molecular side_chains to generate a representative conformation for each; and
- b) generating the CoMFA steric fields for each aligned molecular side_chain.

34. (previously presented) The method of claim 3² further comprising the addition of

topomeric hydrogen bonding fields to the CoMFA steric fields.

5. (canceled)

6. (canceled)

7. (previously presented) A computer implemented method of applying a molecular structural descriptor to the molecular side chains derived from reactant molecules to determine similarity of shape comprising the following steps:

- a) generating standardized representative three dimensional conformations of the molecular side chains derived from reactant molecules comprising the steps of:
 - (1) defining a set of topomeric alignment rules; and
 - (2) applying the topomeric alignment rules to the molecular side chains to generate a representative conformation for each; and
- b) generating the CoMFA steric fields for each topomerically aligned molecular side chain; and
- c) calculating the field differences between all pairs of molecular side chains wherein smaller field differences reflect greater similarity of shape.

8. (previously presented) The method of claim 7 further comprising after step b the additional step of adding topomeric hydrogen bonding fields to the CoMFA fields.

9. (canceled)

10. (canceled)

11. (currently amended) A computer implemented method for configuring the molecular side chains derived from reactant molecules into a standardized representative three

dimensional conformation ~~enabling comparison between the side chains of shape related~~
~~properties~~ enabling comparison of the shape related properties of the side chains, comprising
the following steps:

- a) defining topomeric alignment rules;
- b) obtaining, or generating from two dimensional (2D) structural information, the
three dimensional (3D) configuration of the molecular side chains represented
by the three dimensional coordinates of the atoms comprising the side chains;
and
- c) repositioning the relative positions of the atoms in the side chains by adjusting
torsions according to the topomeric alignment rules

wherein a standardized aligned topomeric conformation is produced for each molecular
side chain.

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12 (currently amended) A computer implemented method of characterizing the three
dimensional structure of the molecular side chains derived from reactant molecules, which can
assume ~~any~~ many conformations, comprising the steps of:

- a) configuring the molecular side chains derived from reactant molecules into a
standardized representative three dimensional conformation comprising the steps
of:
 - (1) defining topomeric alignment rules;
 - (2) obtaining, or generating from two dimensional (2D) structural
information, the three dimensional (3D) configuration of the molecular

side chains represented by the three dimensional coordinates of the atoms comprising the side chains; and

- (3) repositioning the relative positions of the atoms in the side chains by adjusting torsions according to the topomeric alignment rules; and

b) generating the CoMFA steric fields for each aligned molecular side chain.

13. (currently amended) The method of claim 12 further comprising after step ~~b~~ b) the additional step of adding topomeric hydrogen bonding fields to the CoMFA fields.

14. (currently amended) A computer implemented method of applying a molecular structural descriptor to ~~a set of reactants~~ the molecular side chains derived from reactant molecules to determine similarity of shape the molecular side chains derived from reactant molecules to determine similarity of shape comprising the following steps:

- a) configuring the molecular side chains derived from reactant molecules into a standardized representative three dimensional conformation comprising the steps of:
- (1) defining topomeric alignment rules;
 - (2) obtaining, or generating from two dimensional (2D) structural information, the three dimensional (3D) configuration of the molecular side chains represented by the three dimensional coordinates of the atoms comprising the side chains; and
 - (3) repositioning the relative positions of the atoms in the side chains by adjusting torsions according to the topomeric alignment rules; and

- b) generating the CoMFA steric fields for each topomerically aligned molecular side chain; and
- c) calculating the field differences between all pairs of molecular side chains wherein smaller field differences reflect greater similarity of shape.

10 15 (currently amended) The method of claim 1⁹ further comprising after step ~~b~~ b) the additional step of adding topomeric hydrogen bonding fields to the CoMFA fields.